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A New Universality for Random Sequential Deposition of Needles

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Abstract

Percolation and jamming phenomena are investigated for random sequential deposition of rectangular needles on $d = 2$ square lattices. Associated thresholds p_c^{perc} and p_c^{jam} are determined for various needle sizes. Their ratios p_c^{perc}/p_c^{jam} are found to be a constant 0.62 ± 0.01 for all sizes. In addition the ratio of jamming thresholds for respectively square blocks and needles is also found to be a constant 0.79 ± 0.01 . These constants exhibit some universal connexion in the geometry of jamming and percolation for both anisotropic shapes (needles versus square lattices) and isotropic shapes (square blocks on square lattices). A universal empirical law is proposed for all three thresholds as a function of a .

Percolation phenomena are generic in the study of disordered media like porous materials, alloys, ecosystems, etc... [1]. A percolation transition is based on calculating the probability of occurrence of an infinite connectivity between elements of the random medium as a function of the fraction p of constitutive elements. The usually concerned object is the percolating cluster connecting distant borders of the medium. At the critical point p_c^{perc} , this cluster is very tortuous and is a fractal object. Even though some advances have been made in the understanding of percolation, numerous questions remain unanswered today [2]. Among others, the exact values of many thresholds are still not known though some powerful conjectures have been proposed for a rather large class of lattices [3].

Beside connectivity properties, another fundamental question related to disordered structures is the construction of randomly packed structures. Among other models, the random deposition also called Random Sequential Adsorption (RSA), leads to a critical phenomenon. Above a critical fraction p_c^{jam} of occupied sites, the medium becomes fully saturated. No more object can be inserted in it [4]. At this stage the packing density of (identical) objects filling nearly the whole medium is at maximum.

In this paper, we investigate both percolation and jamming phenomena of non-overlapping anisotropic objects (needles) on strictly $d = 2$ square lattices, needles having commensurate scales with respect to the lattice spacing. The study of packed anisotropic objects is relevant for geometrical–physical properties of granular media like the electrical properties of metallic needles [5] or the compaction properties of granules [6]. We will see that both phenomena (percolation and jamming) become highly related to each other independently of the aspect ratio a of the needles.

Earlier studies of needles within the percolation framework have been investigated in the overlapping case only and have been introduced for e.g. mimicking the formation of microfractures in a brittle material [7]. The percolation of non-overlapping needles has never been studied to our knowledge. The RSA of needles has only been considered for specific aspect ratio values, e.g. $a = 2$ on $d = 2$ lattices [8], and for off-lattice cases [9]. It seems that the RSA of needles on discrete lattices has not been considered up to now. The RSA of (isotropic) blocks on a square lattice has been numerically investigated by Nakamura [11] and thereafter confirmed in [12]. We will also compare our work to Nakamura’s result in order to emphasize the effect of anisotropy. Also, an unexpected needle-block relationship will be emphasized

in the following!

On the square lattice, touching needles are needles which have at least one cell side in common. Figure 1 illustrates both percolation and jamming clusters for the particular aspect ratio $a = 4$. The figure presents a 16×16 square lattice at p_c^{perc} and p_c^{jam} for the case of 4×1 needles, and a jammed phase for 4×4 blocks. In the case of needles, one observes that both transitions take place at quite different values of the fraction p of occupied sites. As we will see below, the percolation threshold is “low” implying that the unoccupied sites (holes) can form open and large pores. At the percolation threshold, the needle structure is highly heterogeneous. When the fraction of needles increases, the large pores are filled up to the jamming situation. Near the jamming transition, some short range order appears. Indeed, a close packing of needles oriented in the same direction is observed. Close (oriented) packed needles seem to form blocks of size $a \times a$! In order to emphasize this ordering, a typical jamming phase is presented in Figure 2 for $L = 400$ and for $a = 20$. Horizontal and vertical orientations of needles are represented in different grey levels. The different colors put into evidence the short range ordering. More precisely, some domains of horizontal or vertical needles are seen.

In the third case illustrated in Figure 1, 4×4 blocks are seen in the jamming phase. Large spanning clusters of connected blocks are not formed. One should note that percolation does not occur below the jamming threshold in the case of blocks. However, percolation always takes place before jamming in the case of needles. This makes a big difference between the deposition of anisotropic and isotropic non-overlapping objects on square lattices.

In order to determine the thresholds for both phenomena, numerical simulations have been performed on $d = 2$ square lattices containing up to 2000×2000 sites. Starting from an empty lattice, needles are added sequentially such that p increases linearly. The percolation and jamming phenomena are checked until they are found. The first percolation threshold, i.e. when two distant borders are connected, is considered here, in contrast to the second percolation threshold which is obtained when the four borders are connected [13]. The probability P_{perc} to find a percolating cluster and the probability P_{jam} to find a jamming phase are fitted by the error function

$$P = \frac{1}{\sqrt{2\pi}\Delta} \int_{-\infty}^p \exp \left[-\frac{1}{2} \left(\frac{p' - p_c}{\Delta} \right)^2 \right] dp' \quad (1)$$

where p_c is the critical point and Δ is the width of the transition. Our assumption that the distribution of critical points is a Gaussian is sufficient from a practical point of view, though not claimed to be exact [2]. One should also note that the jamming transition is always sharper than the percolation transition, i.e. $\Delta_{\text{jam}} < \Delta_{\text{perc}}$. The length Δ vanishes [1] as a power of the system size L . One has

$$\Delta \sim L^{-1/\nu} \quad (2)$$

where \sim means asymptotic proportionality. This allows for the measure of the exponent ν for the correlation length ξ which diverges at the critical point as $\xi \sim |p_c - p|^{-\nu}$. The above relationship (2) means that the transition is sharper for larger lattice sizes. As expected, the exponent value has been found to be $\nu_{\text{perc}} = 1.35 \pm 0.02$ compatible with the $\nu_{\text{perc}} = 4/3$ value known for $d = 2$ percolation with isotropic particles. Another exponent value is found for the jamming transition: $\nu_{\text{jam}} = 1.0 \pm 0.1$, a value also reported in the work of Nakamura [11] about the jamming of blocks. Both values ν_{perc} and ν_{jam} have been found to be independent of the aspect ratio a of the needles. It seems at first that both critical phenomena are independent of each other since critical exponents and thresholds are different. However, we will see herebelow that a relationship between percolation and jamming thresholds nevertheless exists!

The threshold values are slightly dependent on the system size L . The following dependence

$$p_c(\infty) - p_c(L) \sim L^{-1/\nu} \quad (3)$$

has been established for percolation [1]. The latter relationship allows us to extrapolate the threshold for an infinite system $L \rightarrow \infty$. Table I summarizes some of the extrapolated values of p_c for both percolation and jamming phenomena for typical values of a . When the aspect ratio a of the needles increases, both thresholds expectedly decrease. Figure 3 presents both p_c^{perc} and p_c^{jam} as a function of a . Curves are guides for the eye.

In order to search for a possible relationship between both thresholds if any, we have calculated the ratio $p_c^{\text{perc}}/p_c^{\text{jam}}$ (see the third column of Table I). Surprisingly, this latter ratio is found to be a constant 0.62 ± 0.01 whatever the aspect ratio value a ! Small deviations from the 0.62 value are only observed for large a values; those deviations are certainly due to the particle/lattice finite size. The universal ratio is unexpected and suggests that both critical phenomena are intimately related, although we have found that

the critical exponent values are different. In fact, this result indicates that the percolation cluster should be a fundamental cluster (like a skeleton) for the jamming phase!

It should be noted that the scaling properties of the jamming phase are not similar to those of dense systems otherwise the threshold p_c^{jam} would be independent of a . In the case of the jamming transition, a power law behavior

$$p_c^{jam} \sim a^{-\delta} \quad (4)$$

with an exponent $\delta \approx 0.20$ has been proposed for off-lattice RSA of rectangles [10]. These authors [10] have suggested that the power law (4) indicates that the network of needles is fractal with a dimension $2-\delta$ at p_c^{jam} at scales below a . Moreover, systematic deviations from Eq.(4) appear for large a values. It seems that both thresholds are decaying in a slower fashion than a power of a (not shown in Figure 3). An empirical law will be proposed in the following.

Consider now the Nakamura work. The ratio between the thresholds p_c^{jam} for blocks and needles seems also to be a universal constant (see the last column of Table I)! This remarkable result suggests that there is also a relationship between needles and blocks for the jamming phase. Of course, we have seen above that close packed needles form clusters which can be seen as blocks of size $a \times a$.

Let us interpret our results by considering a coarse grained view of the disordered systems. In a coarse grained view, i.e. at a scale larger than a , the notion of anisotropy should disappear. Needles of size a are replaced by blocks of size $a \times a$. The threshold is then expected to be that of classical square objects. Since the notion of anisotropy disappears at larger scales, the fraction of occupied sites p' in a coarse grained view is larger than the true fraction of occupied sites p . We propose the equation

$$p = p' \left[1 - \gamma \left(\frac{a-1}{a} \right)^2 \right] \quad (5)$$

where γ is a constant. The factor in the r.h.s. represents the fraction of free sites remaining if two perpendicular needles are touching in any $a \times a$ “supersite”. This term represents the loss of information when one looks for the connectivity of the packing in a coarse grained view. This term represents also the jamming phase since no more needles can be added in a “supersite” which contains already 2 perpendicular touching needles. The parameter γ

should depend only on geometrical aspects and should be independent of a . Using the relationship (5), one expects that both thresholds scale as

$$p_c(a) = C \left[1 - \gamma \left(\frac{a-1}{a} \right)^2 \right] \quad (6)$$

where C is a constant. The law (6) fits the data and is illustrated in Figure 4. The agreement is quite remarkable. The coefficient γ is found: $\gamma = 0.31 \pm 0.01$ in all cases, providing a constant ratio of thresholds. One should note that the Eq.(6) is not valid for $a = 1$ which is a particular (isotropic needles!) point.

In the Nakamura case (blocks of size a), one has a loss of information due to block edges. The empirical law of Eq.(6) is found to hold also in that case! This good agreement suggests that our physical arguments are appropriate to the study of packed anisotropic objects.

In summary, we have investigated two phenomena, i.e. percolation and jamming, which have been independently studied up to now. We have found that they are closely related in the case of anisotropic objects (needles). We have interpreted this effect assuming a loss of information in a coarse grained view. Fundamental laws have been obtained theoretically. Finite size and shape effects seem to have been captured in a scaling law of $(1 - 1/a)^2$ for needles.

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a	needles			p_c^{jam}	$\frac{p_c^{jam}(blocks)}{p_c^{jam}(needles)}$
	p_c^{perc}	p_c^{jam}	$\frac{p_c^{perc}}{p_c^{jam}}$		
2	0.562	0.906	0.621	0.749	0.827
3	0.528	0.847	0.623	0.681	0.804
4	0.504	0.811	0.622	0.646	0.797
5	0.490	0.787	0.623	0.628	0.798
6	0.479	0.770	0.622	0.620	0.805
8	0.474	0.757	0.626	0.603	0.797
10	0.467	0.741	0.630	0.593	0.800

Table I — List of some thresholds p_c for both percolation and jamming phenomena for typical values of the needle aspect ratio a . The ratio p_c^{perc}/p_c^{jam} is also given in the fourth column. The Nakamura thresholds for blocks in the jamming phase are given in the fifth column. In that case, a represents the block width. The last column gives the ratios for blocks and needles thresholds p_c^{jam} .

Figure captions

Figure 1 — (a) Percolation cluster of non-overlapping needles of aspect ratio $a = 4$. (b) The largest cluster at the jamming transition.

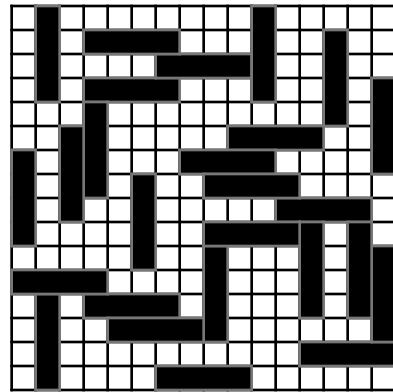
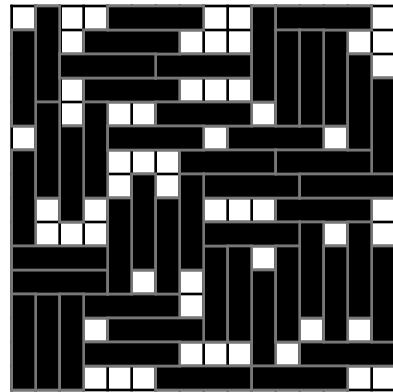
Figure 2 — Jamming phase for $a = 20$ needles. The lattice size is 500×500 . Vertical and horizontal orientations are represented by different grey levels.

Figure 3 — The thresholds p_c^{perc} and p_c^{jam} as a function of the needle aspect ratio a . The nakamura results are also illustrated. The curves are only guides for the eye.

Figure 4 — The thresholds p_c^{perc} and p_c^{jam} as a function of $(a - 1)^2/a^2$. The Nakamura results are also illustrated. The straight lines are fits using Eq.(6).

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p_c^{perc}  p_c^{jam}  p_c^{jam} 